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14. ABSTRACT
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Numerous authors who simulated RTD with the Wigner-Poisson model assumed that the discrete Wigner function is periodic in momentum space. The periodicity follows from the Fourier transform of the density matrix. The inverse Fourier transform provides us with the important proof that the number of spatial intervals is equal to the number of intervals in the momentum space. In addition we obtain that the step size in the momentum space does not depend on the number of intervals. As a result the number of relevant intervals in the momentum space does not also depend on the total number of intervals. Stability of algorithms used by different authors is investigated. The analysis of the stability shows that Greg Recine has used unstable algorithm.

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NAME	PERCENT_SUPPORTED	National Academy Member
Igor Sizov	0.10	
Tatiana Globus	0.20	
Boris Gelmont	0.70	
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Scientific Progress

Fundamental research in the area of solid-state devices is a corner stone and an essential requirement for the development of future electronic systems with relevance to military defense. In order to offer superior capabilities, these systems will need to operate at much higher speeds and frequencies, have greatly increased functionality, and have much higher levels of integration

than present day technology provides. Resonant tunneling diodes (RTDs) have been of interest to the physics and engineering communities since the 1980s because they are inherently high-speed devices. For example, an RTD-based fundamental oscillator achieved the highest frequency generated by a solid-state source (> 700 GHz) in 1991 [1]. The simulation a resonant-tunneling diode (RTD) can be made in different ways. The first successful approach was made solving the Schrodinger equation and calculating the transmission of a diode. However there is a problem how to include the scattering processes in quantum mechanical simulation a resonant-tunneling diode . The Green function method has been one of alternatives. Another alternative was to utilize the Wigner function. The Wigner function approach to the simulation of a resonant-tunneling diode offers many advantages. In the limit of the classical physics the Wigner equation turns into the Boltzmann equation . The scattering processes can be presented in the similar way as in the Boltzmann equation . A short review of simulations made by different authors using the Wigner formalism can be found in [2]. The Wigner function equation was first employed in quantum device simulation by Frensley [3]. Later, Kluksdahl et al [4] incorporated Poisson's equation (PE)and applied the model to the study of RTD with self-consistent potentials. They have chosen Lax-Wendroff explicit time differencing. Jensen, and Buot [5] have used Cayley time evolution operator.

Recent work has focused on solving the time-dependent Wigner-Poisson equations to look for oscillatory solutions. Several groups have studied dynamical instabilities and undertaken the simulation the RTD time-dependent behavior using the discrete Wigner function approach to look for oscillatory solutions [5-10]. However there are also difficulties in applications of the Wigner formalism. It is important to recognize that the Wigner function is defined over both real and momentum spaces (i.e., which differs from all other quantum mechanical formalisms) and this significantly increases the theoretical difficulty associated with quantifying the exact requirements on the numerical discretization so as to insure that all necessary physical laws are satisfied (e.g., charge continuity, momentum balance, detailed balance of the equilibrium state, and stability of non-equilibrium states). Furthermore, the more refined numerical solutions of the Wigner-Poisson model yields results in disagreement with prior results that utilized more coarse grained discretizations.

This proposed research project studies the discretization issues associated with the stability and physical accuracy of the numerical solutions to the Wigner-Poisson modeling of resonant tunneling diodes. Here the goal is to establish the qualitative and quantitative requirements for the phase space discretizations that will be able to generate physically accurate numerical solutions to the Wigner-Poisson model for open systems. The goals of this project is also to study stability and physical accuracy of numerical solutions to the Wigner-Poisson model.

All authors used the discrete Wigner function which is periodic in momentum space. The periodicity was proved from the Fourier transform of the density matrix. The inverse Fourier transform provides us with the important proof that the number of spatial intervals is equal to the number of intervals in the momentum space. In addition we obtain that the step size in the momentum space does not depend on the number of intervals. As a result the number of relevant intervals in the momentum space does not also depend on the total number of intervals.

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Boris Gelmont, Tatiana Globus, Igor Sizov

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The Wigner formalism has previously been applied by numerous groups to analyze the steady-state behavior of particle transport within open quantum systems. In particular, the Wigner-Poisson model has been used as a tool to study electron transport through double-barrier resonant tunneling diodes (RTDs) with open boundary conditions. The goals of this project is to study stability and physical accuracy of numerical solutions to the Wigner-Poisson model. Numerous authors who simulated RTD with the Wigner-Poisson model assumed that the discrete Wigner function is periodic in momentum space. The periodicity follows from the Fourier transform of the density matrix. The inverse Fourier transform provides us with the important proof that the number of spatial intervals is equal to the number of intervals in the momentum space. In addition we obtain that the step size in the momentum space does not depend on the number of intervals. As a result the number of relevant intervals in the momentum space does not also depend on the total number of intervals. Stability of algorithms used by different authors is investigated. The analysis of the stability shows that Greg Recine has used unstable algorithm. .

1.Introduction.

Fundamental research in the area of solid-state devices is a corner stone and an essential requirement for the development of future electronic systems with relevance to military defense. In order to offer superior capabilities, these systems will need to operate at much higher speeds and frequencies, have greatly increased functionality, and have much higher levels of integration than present day technology provides. Resonant tunneling diodes (RTDs) have been of interest to the physics and engineering communities since the 1980s because they are inherently high-speed devices. For example, an RTD-based fundamental oscillator achieved the highest frequency generated by a solid-state source (> 700 GHz) in 1991 [1.1].

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The Wigner function approach to the simulation of a resonant-tunneling diode offers many advantages. In the limit of the classical physics the Wigner equation turns into the Boltzmann equation . The scattering processes can be presented in the similar way as in the Boltzmann equation . A short review of simulations made by different authors using the Wigner formalism can be found in [2].

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However there are also difficulties in applications of the Wigner formalism. It is important to recognize that the Wigner function is defined over both real and momentum spaces (i.e., which differs from all other quantum mechanical formalisms) and this significantly increases the theoretical difficulty associated with quantifying the exact requirements on the numerical discretization so as to insure that all necessary physical laws are satisfied (e.g., charge continuity, momentum balance, detailed balance of the equilibrium state, and stability of non-equilibrium states). Furthermore, the more refined numerical solutions of the Wigner-Poisson model yields results in disagreement with prior results that utilized more coarse grained discretizations.

This proposed research project studies the discretization issues associated with the stability and physical accuracy of the numerical solutions to the Wigner-Poisson modeling of resonant tunneling diodes. Here the goal is to establish the qualitative and quantitative requirements for the phase space discretizations that will be able to generate physically accurate numerical solutions to the Wigner-Poisson model for open systems. The goals of this project is also to study stability and physical accuracy of numerical solutions to the Wigner-Poisson model.

2. Discretization.

Let us consider in more detail a problem of discretization. An equation for the Wigner function can presented as follows

$$\frac{\partial}{\partial t} f(X,k,t) = T(f(X,k,t)) + P(f(X,k,t)) + S(f(X,k,t)) \qquad (1)$$

Here, T represents the kinetic energy for electrons in the device, P represents the potential energy of the electrons, and S the effects of collisions in the device.
In the Wigner-Poisson model eq.(1) has to be solved self consistently with the Poisson equation to account for space charging effect.

The Wigner function, f, is a result of the Weyl- Wigner transform of the density matrix

$$f(X,k) = \int ds \exp(iks) \rho(X + \frac{s}{2}, X - \frac{s}{2}) \qquad (2)$$

It is possible to write reverse transform

$$\frac{1}{2\pi} \int dk \exp(-iks) f(X,k) = \rho(X + \frac{s}{2}, X - \frac{s}{2}) \qquad (3)$$

So the following equation has to be valid

$$f(X,k) = \frac{1}{2\pi} \int dq f(X,q) \int ds \exp(is(k-q)) \qquad (4)$$

If we introduce discretization a fixed spatial with a mesh of we can rewrite this equation as follows

$$f(X,k)=\frac{N_x\Delta x}{2\pi}\int dq f(X,q)\delta_{k,q}=\frac{N_x\Delta x\Delta k}{2\pi}f(X,k) \qquad (5)$$

As a result we have the relationship between momentum and spatial intervals

$$\Delta k\Delta x=\frac{\pi}{N_x} \qquad (6)$$

which was used in all simulations.

The discrete Wigner function is periodic in momentum space, with a period of

$$\frac{\pi\hbar}{\Delta x}=\frac{\pi\hbar N_x}{L} \qquad (7)$$

The spatial interval is equal to

$$\Delta x=\frac{L}{N_x} \qquad (8)$$

Therefore the following relations can be written for momentum interval

$$\Delta k=\frac{\pi N_x}{LN_k} \qquad (9)$$

Hence the maximal wave vector is equal to

$$k_{\max}=\frac{\pi(N_x-1)}{2L} \qquad (10)$$

So it corresponds to the maximal kinetic energy in the momentum space.

$$E_{\max}=\frac{\hbar^2}{2m_n}k_{\max}^2=\frac{\pi^2\hbar^2(N_x-1)^2}{8m_nL^2} \qquad (11)$$

These relations are taken from William R. Frensley]3].

However the more refined numerical solutions of the Wigner-Poisson model yields results in disagreement with prior results that utilized more course grained discretizations. Simulation runs were also performed to show that the size of the momentum mesh can affect the

shape of the steady-state current -voltage curve and the shape of the Wigner distribution, but the size of the spatial mesh does not affect either. The left plot of Figure 1 shows results using a fixed spatial mesh of Nx = 513 (where Nx represents a measure of spatial grid points used as was defined earlier) and a variety of momentum meshes, whereas the right plot shows a fixed momentum mesh using Nk = 1024 and various spatial meshes. The maximum value of the current density and the shape of the peaks in the current voltage curve change significantly as the momentum grid were refined, but remain unaffected by changes to the spatial grid.

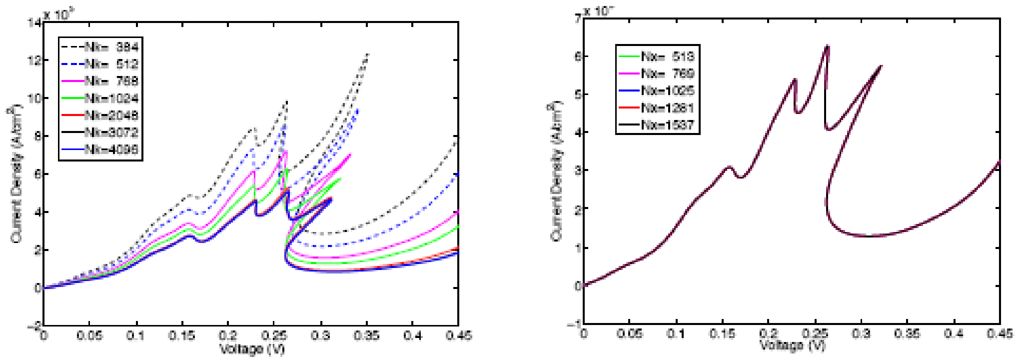

Figure 1. Steady-state IV curves for (left side) fixed spatial mesh, Nx=513, and various momentum meshes, and (right side) fixed momentum mesh, Nk=1024, and various spatial meshes.

However we will be able to demonstrate that the number of both intervals have to be equal to each other if we continue to follow the way which has permitted to us to establish the relationship between momentum and spatial intervals.

A similar derivation can be made for the density matrix. The following equation has to be valid

$$\rho(X+\frac{s}{2},X-\frac{s}{2})=\frac{1}{2\pi}\int d\xi\rho(X+\frac{\xi}{2},X-\frac{\xi}{2})\int dk\exp(ik(\xi-s)) \qquad (12)$$

If we introduce discretization we can rewrite this equation as follows

$$\rho(X+\frac{s}{2},X-\frac{s}{2})=\frac{N_k\Delta k}{2\pi}\int d\xi\rho(X+\frac{\xi}{2},X-\frac{\xi}{2})\delta_{\xi,s}=\frac{N_k\Delta k\Delta x}{2\pi}\rho(X+\frac{s}{2},X-\frac{s}{2}) \quad (13)$$

As a result we have the second relationship between momentum and spatial intervals

$$\Delta k\Delta x=\frac{\pi}{N_k} \qquad (14)$$

Comparing two relationships we have to make a conclusion that momentum and spatial intervals are not independent. The number of spatial intervals is equal to the number of intervals in the momentum space

$$N_k=N_x \qquad (15)$$

In addition we obtain that the step size in the momentum space does not depend on the number of intervals

$$\Delta k = \frac{\pi}{L} \qquad (16)$$

At last a more drastic conclusion has to be made. The maximal energy grows with the increase of the number of intervals. However all variations went to zero before reaching the edges of the wave vector space. As well as the step size in the momentum space does not depend on the number of intervals the number of relevant intervals in the momentum space does not also depend on the total number of intervals. So even in this case it is natural to end simulation at lower values of the wave vector when all variations went to zero before reaching the edges of the wave vector space .

In earlier papers it was taken

$$N_x = 86 \qquad N_k = 72 \quad L = 550A$$

Hence Emax=3.1 eV is too large.

The number of relevant points in the momentum space is possible to estimate if we take the barrier height 0.3 eV as the characteristic value for the end of the variations.

We obtain 26 essential intervals for positive momentums. Hence the number of relevant points is comparable with the total number of points. However the situation is different when the total number of points is large.

$$k_{\max} = \frac{\pi(N_x - 1)}{2L} \qquad (17)$$

grows.

At the same time the number of relevant points in the momentum space

$$\frac{(2m_n V_0)^{1/2}}{\hbar \Delta k} = \frac{(2m_n V_0)^{1/2} L}{\hbar \pi N_x} N_k \qquad (18)$$

remains almost the same .

3. Stability consideration.

A common numerical technique for solving discretized temporal equations is explicit differencing. However an explicit scheme is unconditionally unstable . Stability of the Lax method requires that error in the discretized equation remains bounded. Fourier analysis of the growth of error in these schemes has led to the Courant-Friedrichs-Lewy stability criterion.

$$\Delta t < \frac{v}{\Delta x} \qquad (19)$$

where v is the velocity of the fastest component of the solution.
N. C. Kluksdahl, A. M. Kriman, and D. K. Ferry C. Ringhofer [4] have chosen Lax-Wendroff explicit time differencing. K. L. Jensen and F. A. Buot [54] utilize Cayley time evolution operator. However Greg Recine does not use Cayley time evolution operator. He uses Runge-Kutta type of solver, namely the ROCK4 subroutine. It is known that ROCK4 is an explicit method. Such methods are unstable.

Let us analyze Stability of Cayley time evolution operator. It is enough for this purpose to take into account

$$\hat{T}f = -\frac{\hbar k}{m}\frac{\partial f}{\partial x} = -\frac{\hbar k}{2m\Delta x}\{3f(x) - 4f(x-\Delta x) + f(x-2\Delta x)\} \qquad (20)$$

for k>0
or

$$\hat{T}f = -\frac{\hbar k}{m}\frac{\partial f}{\partial x} = \frac{\hbar k}{2m\Delta x}\{3f(x) - 4f(x+\Delta x) + f(x+2\Delta x)\} \qquad (21)$$

for k<0.

A Cayley time evolution operator will be

$$f(t+\Delta t) = \frac{1+\hat{T}\Delta t/2}{1-\hat{T}\Delta t/2} f(t) \qquad (22)$$

or

$$(1-\hat{T}\Delta t/2) f(t+\Delta t) = (1+\hat{T}\Delta t/2) f(t) \qquad (23)$$

According to von Neuman stability analysis we are looking for the solution as

$$f_j^n = \xi^n \exp(iqj\Delta x) \qquad (24)$$

Hence
for k>0

$$\hat{T}f = -\frac{\hbar k}{2m\Delta x}[1-\exp(-iq\Delta x)][3-\exp(-iq\Delta x)]\xi^n \exp(iqj\Delta x) \qquad (25)$$

Substituting (25) into (23) we obtain

$$\xi^{n+1}\exp(iqj\Delta x)\{1+\frac{\hbar k\Delta t}{4m\Delta x}[1-\exp(-iq\Delta x)][3-\exp(-iq\Delta x)]\} =$$
$$= \xi^n \exp(iqj\Delta x)\{1-\frac{\hbar k\Delta t}{4m\Delta x}[1-\exp(-iq\Delta x)][3-\exp(-iq\Delta x)]\} \qquad (26)$$

We have stable algorithm if an amplitude

$$|\xi|^2 = \{1+4(\frac{\hbar k\Delta t}{2m\Delta x})^2 \sin^2(\frac{q\Delta x}{2})[1+3\sin^2(\frac{q\Delta x}{2})] - \frac{2\hbar k\Delta t}{m\Delta x}\sin^2(\frac{q\Delta x}{2})\cos(\frac{q\Delta x}{2})[1+4\sin^2(\frac{q\Delta x}{2})]\}$$
$$\{1+4(\frac{\hbar k\Delta t}{2m\Delta x})^2 \sin^2(\frac{q\Delta x}{2})[1+3\sin^2(\frac{q\Delta x}{2})] + \frac{2\hbar k\Delta t}{m\Delta x}\sin^2(\frac{q\Delta x}{2})\cos(\frac{q\Delta x}{2})[1+4\sin^2(\frac{q\Delta x}{2})]\}^{-1}$$
(27)
is less than 1 for q< q_{th} where the threshold value of q is equal to
$q_{th} = \pi / \Delta x$ (28)

Similar calculation for k<0 gives
$$|\xi|^2 = \{1+4(\frac{\hbar k\Delta t}{2m\Delta x})^2 \sin^2(\frac{q\Delta x}{2})[1+3\sin^2(\frac{q\Delta x}{2})] + \frac{2\hbar k\Delta t}{m\Delta x}\sin^2(\frac{q\Delta x}{2})\cos(\frac{q\Delta x}{2})[1+4\sin^2(\frac{q\Delta x}{2})]\}$$
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(29)

It follows from our solution that there is instability at large q at any time step.
It is interesting that the threshold value of q does not depend on k.
Let us compare with Lax method.

$$\frac{1}{\Delta t}[f_j^{n+1} - \frac{1}{2}(f_{j+1}^n + f_{j-1}^n)] = -\frac{\hbar k}{2m\Delta x}(f_{j+1}^n - f_{j-1}^n) \quad (30)$$

or

$$f_j^{n+1} = \frac{1}{2}(f_{j+1}^n + f_{j-1}^n) - \frac{\hbar k\Delta t}{2m\Delta x}(f_{j+1}^n - f_{j-1}^n) \quad (31)$$

According to von Neuman stability analysis we have

$$\xi = \cos(q\Delta x) - \frac{i\hbar k\Delta t}{m\Delta x}\sin(q\Delta x) \quad (32)$$

The magnitude is equal to

$$|\xi|^2 = \cos^2(q\Delta x) + (\frac{\hbar k\Delta t}{m\Delta x})^2 \sin^2(q\Delta x) = 1 - (\frac{\hbar k\Delta t}{m\Delta x})^2 \cos^2(q\Delta x) \quad (33)$$

We have as a result Courant-Friedrichs-Lewy stability criterion

$$\Delta t < \frac{m\Delta x}{\hbar k} \quad (33)$$

which does not depend on q but depends on k.

4.Conclusion.

All authors used the discrete Wigner function which is periodic in momentum space. The periodicity was proved from the Fourier transform of the density matrix. The inverse Fourier transform provides us with the important proof that the number of spatial intervals is equal to the number of intervals in the momentum space. In addition we obtain that the step size in the momentum space does not depend on the number of intervals. As a result the number of relevant intervals in the momentum space does not also depend on the total number of intervals.

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